



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:17 PM EST

PDB ID : 1TUF
Title : Crystal structure of Diaminopimelate Decarboxylase from *m. jannaschi*
Authors : Rajashankar, K.; Ray, S.R.; Bonanno, J.B.; Pinho, M.G.; He, G.; De Lencastre, H.; Tomasz, A.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-06-24
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

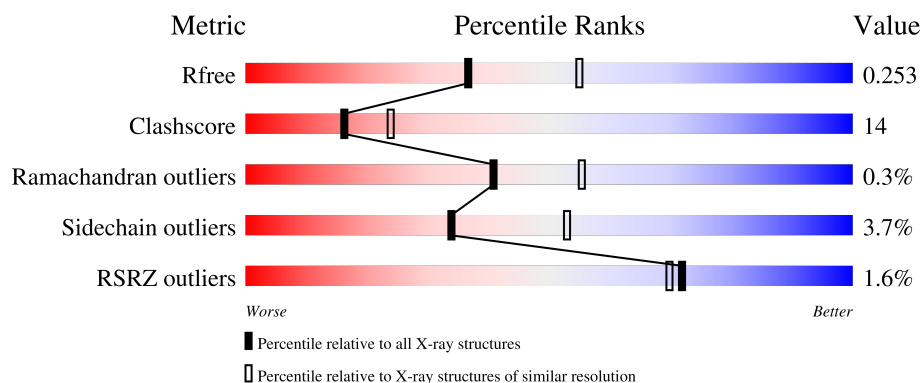
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>30%</div> <div>.</div> </div> </div>
1	B	434	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7142 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

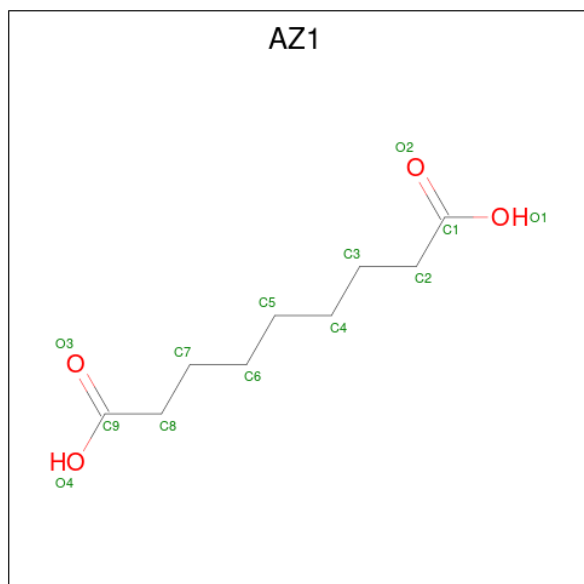
- Molecule 1 is a protein called Diaminopimelate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	P	S	0	0	0
			3412	2178	569	644	1	20			
1	B	434	Total	C	N	O	P	S	0	0	0
			3412	2178	569	644	1	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	LLP	LYS	modified residue	UNP Q58497
B	83	LLP	LYS	modified residue	UNP Q58497

- Molecule 2 is AZELAIC ACID (three-letter code: AZ1) (formula: C₉H₁₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	9	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	9	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	179	Total	O	0	0
			179	179		

- Molecule 1: Diaminopimelate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	80.81Å 80.81Å 508.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 29.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.3 (25.00-2.40) 88.4 (29.24-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.253 0.203 , 0.253	Depositor DCC
R_{free} test set	1804 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.496	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7142	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AZ1, LLP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.36	0/3445	0.59	0/4646
1	B	0.37	0/3445	0.61	0/4646
All	All	0.36	0/6890	0.60	0/9292

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3412	0	3462	122	0
1	B	3412	0	3461	97	0
2	A	13	0	14	1	0
2	B	13	0	14	0	0
3	A	113	0	0	1	0
3	B	179	0	0	3	0
All	All	7142	0	6951	199	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:LEU:HD21	1:A:412:ARG:HD2	1.44	0.97
1:B:407:ASN:HD22	1:B:409:TYR:H	1.22	0.86
1:A:407:ASN:HD22	1:A:409:TYR:H	1.24	0.85
1:A:175:PRO:HB3	1:A:241:LYS:HB3	1.61	0.82
1:A:316:LEU:HB3	1:A:395:ILE:CG2	2.14	0.77
1:B:316:LEU:HB3	1:B:395:ILE:HG23	1.68	0.76
1:A:113:LYS:HE2	1:A:113:LYS:HA	1.69	0.75
1:A:153:LEU:HD11	1:A:210:ALA:HB2	1.68	0.74
1:B:371:LEU:HD21	1:B:412:ARG:HD3	1.70	0.72
1:A:47:TYR:HB2	1:A:417:MET:HG2	1.72	0.72
1:B:250:LYS:HG3	1:B:296:VAL:HG22	1.72	0.71
1:B:19:ASP:H	1:B:53:GLN:HE22	1.39	0.71
1:A:338:MET:HG2	1:A:371:LEU:HD12	1.73	0.70
1:A:420:THR:HG22	1:A:425:VAL:HG12	1.71	0.70
1:B:232:ILE:HD11	1:B:281:LEU:HA	1.75	0.68
1:A:267:ILE:HD11	1:A:308:SER:HA	1.75	0.68
1:B:182:HIS:HB3	1:B:185:ILE:HD13	1.76	0.68
1:A:343:ARG:HD3	1:A:351:HIS:NE2	2.10	0.67
1:A:371:LEU:CD2	1:A:412:ARG:HD2	2.20	0.67
1:A:220:GLY:HA2	1:A:256:ILE:HG23	1.77	0.67
1:A:233:SER:HB3	1:A:234:PRO:HD3	1.76	0.67
1:A:224:HIS:HD2	1:A:263:GLY:H	1.41	0.66
1:B:407:ASN:ND2	1:B:409:TYR:H	1.92	0.66
1:B:326:THR:HB	1:B:327:PRO:HD2	1.78	0.64
1:A:157:ASN:ND2	1:A:213:MET:HB3	2.12	0.64
1:B:343:ARG:HB3	1:B:344:PRO:HD3	1.78	0.64
1:A:414:ARG:NH2	1:B:408:ASN:HD22	1.96	0.64
1:B:303:LEU:C	1:B:305:PRO:HD3	2.17	0.64
1:A:417:MET:HB2	1:A:429:ARG:HB3	1.79	0.64
1:B:157:ASN:HD21	1:B:215:TYR:H	1.46	0.63
1:A:407:ASN:ND2	1:A:409:TYR:H	1.95	0.62
1:B:243:MET:HE3	1:B:259:VAL:HG11	1.82	0.62
1:A:15:PHE:N	1:A:18:ASN:HD22	1.97	0.61
1:A:243:MET:HE1	1:A:246:VAL:HG21	1.82	0.61
1:A:320:VAL:HG12	1:A:391:ASP:O	2.01	0.61
1:A:267:ILE:HD11	1:A:308:SER:CA	2.31	0.60
1:A:244:ASP:O	1:A:247:VAL:HG22	2.01	0.60
1:A:408:ASN:ND2	1:B:414:ARG:NH2	2.49	0.60
1:A:343:ARG:HB3	1:A:344:PRO:HD3	1.85	0.59
1:A:16:LEU:HD22	1:A:268:PRO:HB3	1.83	0.59
1:A:33:TYR:OH	1:A:424:GLY:HA2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG21	1:B:372:CYS:HB2	1.83	0.59
1:A:267:ILE:HD13	1:A:307:ARG:HD2	1.83	0.59
1:A:23:ILE:HD11	1:A:358:VAL:HG21	1.85	0.58
1:A:408:ASN:ND2	1:B:414:ARG:HH22	1.99	0.58
1:A:211:LEU:HD21	1:A:218:VAL:HG21	1.85	0.58
1:B:330:LYS:HD3	1:B:365:VAL:HG12	1.86	0.58
1:A:303:LEU:C	1:A:305:PRO:HD3	2.23	0.57
1:A:231:ASP:O	1:A:234:PRO:HD2	2.04	0.57
1:A:408:ASN:HD22	1:B:414:ARG:NH2	2.03	0.57
1:B:371:LEU:CD2	1:B:412:ARG:HD3	2.34	0.56
1:A:340:ASP:OD1	1:A:415:PRO:HD3	2.05	0.56
1:B:267:ILE:HD11	1:B:269:TYR:CE1	2.40	0.56
1:B:341:MET:HE1	1:B:344:PRO:HD3	1.87	0.56
1:A:157:ASN:HD22	1:A:216:VAL:HG13	1.69	0.56
1:B:383:GLU:C	1:B:384:LEU:HD23	2.26	0.56
1:B:182:HIS:CD2	1:B:234:PRO:HG3	2.41	0.55
1:B:92:ARG:HH11	1:B:115:SER:HA	1.72	0.55
1:A:134:ILE:HD12	1:A:155:LEU:HD13	1.89	0.55
1:B:157:ASN:HD22	1:B:216:VAL:HG13	1.72	0.54
1:A:412:ARG:HD3	3:A:534:HOH:O	2.08	0.54
1:B:233:SER:HB3	1:B:234:PRO:HD3	1.90	0.53
1:A:322:HIS:CE1	1:B:155:LEU:HD12	2.42	0.53
1:A:62:ILE:HG22	1:A:66:LYS:HE3	1.91	0.53
1:B:371:LEU:CD2	1:B:412:ARG:CD	2.87	0.53
1:A:243:MET:HE2	1:A:243:MET:HA	1.90	0.52
1:B:149:SER:HA	1:B:196:LEU:HD21	1.91	0.52
1:B:204:MET:HE2	1:B:208:LYS:HG3	1.91	0.52
1:A:250:LYS:HG3	1:A:296:VAL:HG12	1.91	0.52
1:A:444:PRO:HD2	1:A:447:LEU:HD12	1.91	0.52
1:B:220:GLY:HA2	1:B:256:ILE:HG23	1.90	0.52
1:A:104:VAL:HG21	1:B:372:CYS:SG	2.50	0.52
1:B:92:ARG:NH1	1:B:114:LEU:O	2.42	0.52
1:B:410:ASN:N	1:B:410:ASN:HD22	2.07	0.52
1:B:408:ASN:HA	1:B:412:ARG:O	2.10	0.52
1:B:213:MET:HB2	1:B:216:VAL:HG22	1.92	0.51
1:A:326:THR:HB	1:A:327:PRO:HD2	1.92	0.51
1:B:66:LYS:O	1:B:70:GLU:HG3	2.10	0.51
1:A:224:HIS:CD2	1:A:263:GLY:H	2.26	0.51
1:A:414:ARG:HD3	1:A:432:GLU:OE1	2.10	0.51
1:A:411:ALA:HB3	1:B:108:GLU:HG2	1.92	0.50
1:B:408:ASN:OD1	1:B:413:GLY:HA2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HH22	2:A:502:AZ1:H22	1.76	0.50
1:B:341:MET:HE2	1:B:398:VAL:HG12	1.93	0.50
1:B:414:ARG:HD3	1:B:432:GLU:OE1	2.12	0.50
1:A:155:LEU:HD12	1:B:322:HIS:CE1	2.47	0.50
1:A:332:VAL:HG11	1:A:393:LEU:HD11	1.94	0.50
1:A:243:MET:CE	1:A:246:VAL:HG21	2.42	0.50
1:A:367:ILE:N	1:A:367:ILE:HD12	2.27	0.50
1:A:88:LEU:O	1:A:92:ARG:HB2	2.12	0.49
1:B:153:LEU:HD11	1:B:210:ALA:HB2	1.94	0.49
1:B:371:LEU:HD21	1:B:412:ARG:CD	2.42	0.49
1:B:88:LEU:O	1:B:92:ARG:HB2	2.13	0.49
1:A:321:HIS:HD2	3:B:551:HOH:O	1.94	0.49
1:B:130:THR:OG1	1:B:133:GLU:HG3	2.12	0.49
1:B:338:MET:HG2	1:B:371:LEU:HD12	1.95	0.49
1:A:368:ALA:HB1	1:B:193:LYS:HD3	1.94	0.49
1:A:385:ASP:O	1:A:386:LYS:C	2.52	0.49
1:B:434:TYR:HA	1:B:437:LEU:HD23	1.95	0.49
1:A:316:LEU:HB3	1:A:395:ILE:HG22	1.94	0.49
1:A:155:LEU:HD12	1:B:322:HIS:HE1	1.78	0.49
1:A:408:ASN:HA	1:A:412:ARG:O	2.13	0.48
1:A:130:THR:OG1	1:A:133:GLU:HG3	2.13	0.48
1:A:266:GLY:C	1:A:267:ILE:HD12	2.34	0.48
1:A:407:ASN:HB2	3:B:572:HOH:O	2.13	0.48
1:B:310:VAL:HG23	1:B:400:ALA:HB2	1.96	0.48
1:B:338:MET:CG	1:B:371:LEU:HD12	2.43	0.48
1:A:414:ARG:NH2	1:B:408:ASN:ND2	2.62	0.47
1:A:213:MET:HB2	1:A:216:VAL:HG22	1.96	0.47
1:A:79:ALA:O	1:A:304:GLU:HA	2.14	0.47
1:A:295:LYS:HB3	1:A:295:LYS:HZ2	1.79	0.47
1:B:290:LEU:O	1:B:293:LYS:HG2	2.14	0.47
1:B:413:GLY:HA3	1:B:432:GLU:HB2	1.96	0.47
1:A:321:HIS:CE1	1:A:335:ASP:HB3	2.49	0.47
1:A:371:LEU:HD22	1:A:410:ASN:HB2	1.96	0.47
1:B:127:ASN:ND2	1:B:193:LYS:HD2	2.30	0.47
1:A:176:ASN:HD21	1:A:199:GLU:HG3	1.79	0.47
1:A:414:ARG:HH22	1:B:408:ASN:ND2	2.13	0.47
1:A:417:MET:O	1:A:427:LEU:HD12	2.15	0.47
1:B:103:VAL:HB	1:B:108:GLU:HB2	1.97	0.47
1:A:316:LEU:HB3	1:A:395:ILE:HG23	1.96	0.46
1:A:173:ILE:O	1:A:175:PRO:HD3	2.16	0.46
1:A:178:ASN:OD1	1:A:180:LYS:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TYR:CB	1:A:417:MET:HG2	2.44	0.46
1:A:104:VAL:HG21	1:B:372:CYS:CB	2.46	0.46
1:B:285:ILE:O	1:B:289:MET:HG2	2.16	0.46
1:B:177:VAL:HG13	1:B:237:GLU:OE1	2.16	0.45
1:A:238:GLU:O	1:A:242:VAL:HG23	2.15	0.45
1:B:228:GLN:HA	1:B:266:GLY:HA2	1.98	0.45
1:A:61:TYR:CD2	1:A:278:GLN:HG2	2.52	0.45
1:A:88:LEU:HD13	1:B:443:VAL:HG23	1.99	0.45
1:A:88:LEU:HD13	1:B:443:VAL:CG2	2.47	0.45
1:B:119:SER:HA	1:B:122:ILE:HD12	1.98	0.45
1:A:120:LYS:O	1:A:120:LYS:HG2	2.15	0.45
1:A:172:ARG:HA	1:A:222:HIS:O	2.16	0.45
1:B:231:ASP:O	1:B:234:PRO:HD2	2.16	0.45
1:A:153:LEU:HD22	1:A:213:MET:SD	2.57	0.45
1:A:249:LEU:HD13	1:A:256:ILE:HD11	1.97	0.45
1:B:401:TYR:HB3	1:B:405:MET:CE	2.47	0.45
1:A:414:ARG:HH22	1:B:408:ASN:HD22	1.63	0.45
1:B:257:GLU:O	1:B:299:PRO:HB2	2.17	0.45
1:B:52:GLU:HG2	3:B:597:HOH:O	2.17	0.45
1:A:127:ASN:HD22	1:B:333:MET:CE	2.30	0.45
1:A:338:MET:CG	1:A:371:LEU:HD12	2.44	0.44
1:B:211:LEU:HD11	1:B:254:ILE:HG12	1.99	0.44
1:A:295:LYS:HB3	1:A:295:LYS:NZ	2.33	0.44
1:A:119:SER:HA	1:A:122:ILE:HD12	1.99	0.44
1:A:329:THR:HG22	1:A:330:LYS:N	2.32	0.44
1:B:268:PRO:HD3	1:B:275:ILE:HD11	1.98	0.44
1:A:218:VAL:HG23	1:A:218:VAL:O	2.18	0.43
1:A:23:ILE:O	1:A:23:ILE:HG23	2.18	0.43
1:A:74:LYS:HG3	1:A:298:MET:O	2.18	0.43
1:A:66:LYS:O	1:A:70:GLU:HG3	2.19	0.43
1:A:38:LEU:HD21	1:A:425:VAL:HG11	2.01	0.43
1:A:193:LYS:HD3	1:B:368:ALA:HB1	2.00	0.43
1:A:219:VAL:O	1:A:257:GLU:HB3	2.18	0.43
1:B:340:ASP:OD1	1:B:415:PRO:HD3	2.19	0.43
1:A:134:ILE:CD1	1:A:155:LEU:HD13	2.49	0.43
1:B:258:ASP:OD1	1:B:300:ASN:HB2	2.18	0.43
1:B:174:ASN:HB3	1:B:189:LEU:HB3	2.01	0.43
1:B:33:TYR:OH	1:B:424:GLY:HA2	2.19	0.43
1:A:290:LEU:C	1:A:292:TYR:H	2.23	0.43
1:A:286:ILE:O	1:A:290:LEU:HG	2.19	0.43
1:A:347:TYR:O	1:A:348:GLU:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:VAL:HG12	1:B:125:ASN:HB2	2.00	0.43
1:A:152:GLU:O	1:A:156:ILE:HG13	2.18	0.42
1:A:311:ALA:O	1:A:397:ASP:HA	2.19	0.42
1:A:157:ASN:HD21	1:A:215:TYR:H	1.68	0.42
1:B:251:GLU:HG2	1:B:295:LYS:NZ	2.34	0.42
1:B:177:VAL:HA	1:B:241:LYS:HZ2	1.84	0.42
1:A:62:ILE:O	1:A:66:LYS:HG3	2.19	0.42
1:B:250:LYS:CG	1:B:296:VAL:HG22	2.44	0.42
1:B:304:GLU:N	1:B:305:PRO:HD3	2.33	0.42
1:B:401:TYR:O	1:B:405:MET:HE2	2.19	0.42
1:A:416:ARG:HG2	1:A:427:LEU:HD11	2.02	0.42
1:A:69:GLU:HG3	1:A:74:LYS:O	2.20	0.42
1:B:47:TYR:HB2	1:B:417:MET:HG2	2.01	0.41
1:B:19:ASP:N	1:B:53:GLN:HE22	2.13	0.41
1:B:232:ILE:HD11	1:B:281:LEU:CA	2.48	0.41
1:A:321:HIS:HE1	1:A:335:ASP:OD2	2.03	0.41
1:B:296:VAL:HG12	1:B:297:GLU:N	2.34	0.41
1:A:228:GLN:O	1:A:228:GLN:HG3	2.20	0.41
1:A:304:GLU:N	1:A:305:PRO:HD3	2.35	0.41
1:A:371:LEU:HD22	1:A:410:ASN:CB	2.50	0.41
1:B:359:LYS:H	1:B:385:ASP:HB3	1.84	0.41
1:B:228:GLN:HG3	1:B:228:GLN:O	2.21	0.41
1:A:29:PHE:HA	1:A:33:TYR:O	2.20	0.41
1:B:385:ASP:O	1:B:386:LYS:C	2.59	0.41
1:A:267:ILE:HA	1:A:268:PRO:HD3	1.84	0.41
1:B:267:ILE:HD13	1:B:311:ALA:HB1	2.02	0.41
1:A:343:ARG:NH1	1:A:349:ALA:HB1	2.36	0.41
1:A:380:ARG:HG3	1:A:380:ARG:HH11	1.85	0.41
1:A:417:MET:HB2	1:A:429:ARG:CB	2.47	0.41
1:B:361:GLU:HG3	1:B:386:LYS:CG	2.51	0.41
1:A:380:ARG:NH1	1:A:380:ARG:HG3	2.37	0.40
1:B:320:VAL:HG12	1:B:391:ASP:O	2.21	0.40
1:A:411:ALA:HB3	1:B:108:GLU:CG	2.51	0.40
1:B:125:ASN:CG	1:B:146:ASN:HD22	2.25	0.40
1:A:228:GLN:HA	1:A:266:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	431/434 (99%)	410 (95%)	20 (5%)	1 (0%)	47	62
1	B	431/434 (99%)	413 (96%)	16 (4%)	2 (0%)	29	41
All	All	862/868 (99%)	823 (96%)	36 (4%)	3 (0%)	41	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	GLY
1	B	85	ASN
1	B	181	THR

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/366 (100%)	353 (96%)	13 (4%)	35	54
1	B	366/366 (100%)	352 (96%)	14 (4%)	33	51
All	All	732/732 (100%)	705 (96%)	27 (4%)	34	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	109	LEU
1	A	116	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	124	PHE
1	A	153	LEU
1	A	155	LEU
1	A	294	ASP
1	A	295	LYS
1	A	299	PRO
1	A	372	CYS
1	A	385	ASP
1	A	407	ASN
1	A	410	ASN
1	B	16	LEU
1	B	88	LEU
1	B	109	LEU
1	B	124	PHE
1	B	153	LEU
1	B	155	LEU
1	B	299	PRO
1	B	333	MET
1	B	372	CYS
1	B	395	ILE
1	B	407	ASN
1	B	410	ASN
1	B	414	ARG
1	B	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	127	ASN
1	A	141	ASN
1	A	157	ASN
1	A	176	ASN
1	A	192	ASN
1	A	217	ASN
1	A	224	HIS
1	A	321	HIS
1	A	407	ASN
1	A	408	ASN
1	B	18	ASN
1	B	53	GLN
1	B	141	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ASN
1	B	157	ASN
1	B	192	ASN
1	B	217	ASN
1	B	321	HIS
1	B	407	ASN
1	B	408	ASN
1	B	410	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	LLP	A	83	1	23,24,25	2.15	7 (30%)	25,32,34	2.22	7 (28%)
1	LLP	B	83	1	23,24,25	1.97	6 (26%)	25,32,34	2.18	6 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	83	1	-	5/16/17/19	0/1/1/1
1	LLP	B	83	1	-	5/16/17/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	LLP	C4-C4'	5.56	1.57	1.46
1	B	83	LLP	C4-C4'	4.90	1.55	1.46
1	A	83	LLP	C4-C5	4.43	1.47	1.42
1	B	83	LLP	C4-C5	4.22	1.47	1.42
1	B	83	LLP	C2-N1	3.99	1.41	1.33
1	A	83	LLP	C2-N1	3.63	1.40	1.33
1	A	83	LLP	C4'-NZ	2.92	1.37	1.27
1	A	83	LLP	P-OP3	-2.42	1.45	1.54
1	A	83	LLP	C6-N1	2.41	1.39	1.34
1	B	83	LLP	C4'-NZ	2.40	1.35	1.27
1	A	83	LLP	C3-C2	2.36	1.43	1.40
1	B	83	LLP	C6-N1	2.20	1.39	1.34
1	B	83	LLP	P-OP3	-2.20	1.46	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	LLP	C2'-C2-C3	5.48	127.66	120.89
1	B	83	LLP	CE-NZ-C4'	5.47	135.69	118.90
1	A	83	LLP	CE-NZ-C4'	5.38	135.43	118.90
1	B	83	LLP	C2'-C2-C3	4.99	127.05	120.89
1	B	83	LLP	C4-C4'-NZ	-4.08	105.57	124.31
1	A	83	LLP	OP4-C5'-C5	3.85	116.69	109.35
1	A	83	LLP	C4-C4'-NZ	-3.84	106.70	124.31
1	B	83	LLP	OP4-C5'-C5	3.83	116.66	109.35
1	B	83	LLP	C4-C3-C2	3.50	122.36	120.19
1	A	83	LLP	C4-C3-C2	3.32	122.24	120.19
1	A	83	LLP	C5'-C5-C6	-2.62	115.06	119.37
1	B	83	LLP	C5'-C5-C6	-2.36	115.49	119.37
1	A	83	LLP	C3-C2-N1	-2.05	118.12	120.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	83	LLP	C4-C4'-NZ-CE
1	B	83	LLP	C4-C4'-NZ-CE
1	A	83	LLP	CG-CD-CE-NZ
1	B	83	LLP	CG-CD-CE-NZ
1	B	83	LLP	C5-C4-C4'-NZ
1	A	83	LLP	CE-CD-CG-CB
1	B	83	LLP	C3-C4-C4'-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	A	83	LLP	C3-C4-C4'-NZ
1	A	83	LLP	C5-C4-C4'-NZ
1	B	83	LLP	CE-CD-CG-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	AZ1	B	503	-	6,12,12	0.55	0	5,13,13	2.96	3 (60%)
2	AZ1	A	502	-	6,12,12	0.34	0	5,13,13	2.88	4 (80%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AZ1	B	503	-	-	4/6/10/10	-
2	AZ1	A	502	-	-	3/6/10/10	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	AZ1	C4-C3-C2	4.64	131.82	113.76
2	A	502	AZ1	C4-C3-C2	4.57	131.53	113.76
2	B	503	AZ1	C7-C6-C5	3.26	131.00	114.42
2	A	502	AZ1	C7-C6-C5	3.14	130.39	114.42
2	B	503	AZ1	C6-C7-C8	2.75	124.45	113.76
2	A	502	AZ1	C6-C7-C8	2.52	123.59	113.76
2	A	502	AZ1	C5-C4-C3	2.06	124.86	114.42

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	AZ1	C2-C3-C4-C5
2	B	503	AZ1	C5-C6-C7-C8
2	A	502	AZ1	C4-C5-C6-C7
2	B	503	AZ1	C2-C3-C4-C5
2	A	502	AZ1	C3-C4-C5-C6
2	B	503	AZ1	C6-C7-C8-C9
2	B	503	AZ1	C4-C5-C6-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	AZ1	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	433/434 (99%)	-0.13	6 (1%) 75 73	24, 40, 62, 74	0
1	B	433/434 (99%)	-0.35	8 (1%) 68 66	23, 35, 56, 82	0
All	All	866/868 (99%)	-0.24	14 (1%) 72 70	23, 37, 61, 82	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	ASN	4.0
1	A	360	ASN	3.8
1	A	180	LYS	3.7
1	B	183	PRO	3.5
1	B	179	PRO	3.3
1	B	360	ASN	2.9
1	B	180	LYS	2.9
1	A	63	GLU	2.7
1	B	181	THR	2.5
1	A	361	GLU	2.5
1	A	66	LYS	2.4
1	B	188	GLY	2.4
1	A	181	THR	2.3
1	B	187	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	A	83	24/25	0.96	0.20	27,33,38,40	0
1	LLP	B	83	24/25	0.97	0.17	22,32,36,38	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AZ1	B	503	13/13	0.63	0.38	38,42,49,53	0
2	AZ1	A	502	13/13	0.75	0.32	43,45,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.